

# Three Dimensional Ising Model, Percolation Theory and Conformal Invariance

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The fractal structure and scaling properties of a 2d slice of the 3d Ising model is studied using Monte Carlo techniques. The percolation transition of geometric spin (GS) clusters is found to occur at the Curie point, reflecting the critical behavior of the 3d model. The fractal dimension and the winding angle statistics of the perimeter and external perimeter of the geometric spin clusters at the critical point suggest that, if conformally invariant in the scaling limit, they can be described by the theory of Schramm-Löwner evolution (SLE $_{\kappa}$ ) with diffusivity of  $\kappa = 5$  and  $16/5$ , respectively, putting them in the same universality class as the interfaces in 2d tricritical Ising model. It is also found that the Fortuin-Kasteleyn (FK) clusters associated with the cross sections undergo a nontrivial percolation transition, in the same universality class as the ordinary 2d critical percolation.

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Conformal invariance plays the key role in the analytical description of two-dimensional (2d) systems at their critical points [1]. One of the approaches to study the critical behavior of spin models such as  $q$ -state Potts model ( $q \leq 4$ ) is the geometrical approach based on percolation theory [2, 3] and also finite-size scaling (FSS) relations supplied by conformal field theory (CFT) [4, 5]. Fortuin-Kasteleyn (FK) bond representation of Potts model gives a close relation between percolation and thermal phase transition in which critical singularities can be represented in terms of FK clusters [6]. An FK cluster can be constructed from a "geometric" cluster – i.e., a set of nearest neighbor sites of like states, by assigning a bond between each pair of sites with a certain temperature-dependent probability. The FK clusters always percolate right at the critical temperature  $T_c$ . The percolation temperature for both FK and geometric clusters of a  $q$ -state Potts model coincide only in two dimensions.

Critical behavior of the interfaces of these clusters in the scaling limit is conjectured, and in some cases proven, to be described by the theory of Schramm-Löwner evolution (SLE $_{\kappa}$ ) [7]. The diffusivity  $\kappa$  denotes the classification of conformally invariant interfaces whose value for the hull and the external perimeter (EP) of an FK cluster,  $\kappa$  and  $\kappa'$  respectively, satisfy a duality relation  $\kappa\kappa' = 16$  [8] (for a review on SLE, see [9]). Another similar duality also holds in 2d, between the hull of an FK cluster and the hull of a spin cluster. Considering these two duality relations together, one finds that the hull of a spin cluster and the EP of an FK cluster can be described with the same  $\kappa$ . Many connections between SLE and various 2d systems such as turbulence, spin glasses, growth models, sandpile models and disordered Potts model have been recently noticed and discussed [10].

For the Ising model, equivalent to  $q = 2$  Potts model,

in three dimensions (3d) the percolation transition of geometric spin (GS) clusters occurs at some temperature  $T_p$  well below the Curie point  $T_c$  [11]. Thus, contrary to the FK clusters, the 3d geometric clusters do not capture the critical properties of the model. The question that arises is how the FK and GS clusters in a 2d cross sectional slice of the 3d Ising model behave and whether they reflect the critical properties of the 3d model. This is the main subject of the present letter.

In this letter we present the results of extensive Monte Carlo study of 3d Ising model simulated by using Wolff's algorithm [12] based on single cluster update. We examine the FSS hypothesis for some percolation observables on a 2d slice of the lattice, indicating that the percolation threshold of the geometric clusters coincides with the critical point. This is in agreement with the observation of [13], in which the authors have found a power-law scaling behavior in the length distribution of the loops formed by an arbitrary cross section of the boundaries of 3d GS clusters at  $T = T_c$ . In this paper, we undertake a detailed and systematic study of the statistical and percolation properties of all GS clusters on an arbitrary cross section of the system. Note that disjoint GS clusters on a 2d cross section may belong to a 3d GS cluster. The scaling behavior of the GS clusters motivated us to examine possible conformal invariance of the critical geometric clusters which seem to undergo a continuous transition at the threshold. We find that the perimeter and the EP of a GS cluster at the critical point satisfy the duality relation and their fractal dimensions and winding angle statistics are compatible, in the scaling limit, with the family of conformally invariant curves i.e., SLE $_{\kappa}$  with  $\kappa = 5$  and  $16/5$  respectively. This latter is in the same universality class as interfaces in tricritical Ising model in two dimensions.

Our analysis of FK clusters on 2d slices also indicates that these clusters undergo a nontrivial percolation transition at  $\beta_c^{FK}/\beta_c = 1.617(1)$ , in the same universality class as the classical bond percolation.

There exist some numerical investigations of 3d Ising

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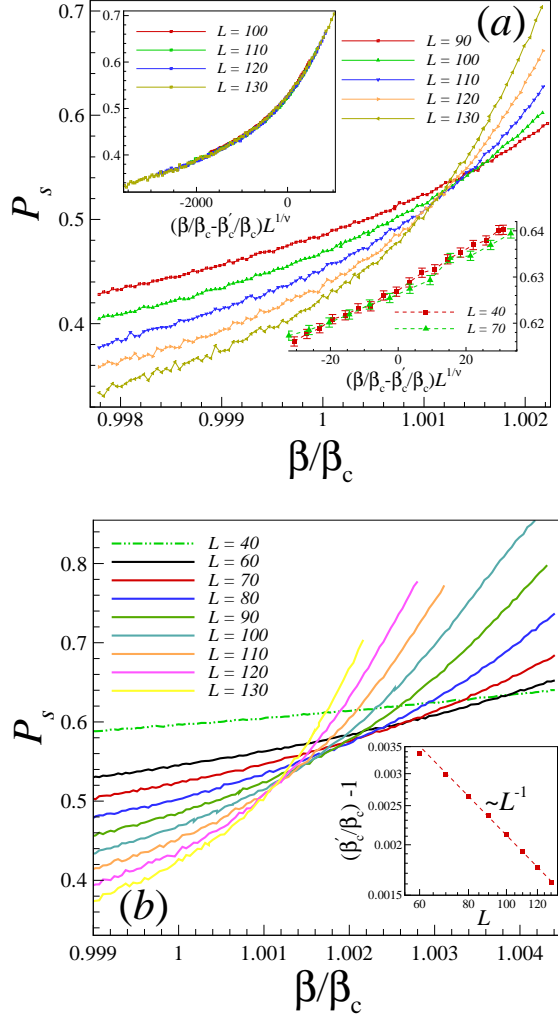


FIG. 1: (Color online) (a) The percolation probability  $P_s$  of GS clusters, measured on 2d cross sections of 3d Ising model of different size  $L^3$ , as a function of  $\beta$ . Upper inset: FSS plots of the data with appropriate values  $\nu = 0.36$  and  $\beta'_c = 1.001172\beta_c$ . Lower inset: the data collapse very close to the crossing point for two  $P_s$  curves of sizes  $L = 40$  and  $70$ , with  $\nu = 0.36$  and  $\beta'_c = 1.003316\beta_c$ . (b) Size dependence of the crossing point  $\beta'_c(L, L')$  of different curves with the reference  $P_s$  curve of  $L' = 40$  (dotted-dashed line).

model on special geometries with specific boundary conditions (bc) [14, 15] which confirm a linear relation between the scaling dimension of the operators of 3d systems and their correlation lengths. This relation has been given by Cardy [16] by exploiting the conformal group transformations.

In order to investigate the fractal structure of the GS clusters on 2d cross sectional slices of 3d Ising model, we first examine the FSS hypothesis for some percolation observables i.e., percolation probability  $P_s$ , percolation strength  $M$ , and the mean cluster size  $\chi$ . For this purpose, the simulation of 3d Ising model is carried out

by using the Wolff's Monte Carlo algorithm [12] on simple cubic (SC) lattices of different size  $L^3$  with free bc, and sizes up to  $L = 150$ . After discarding the first  $L^3$  Monte Carlo sweeps for equilibration, we then analyze the spin configuration of a planar slice of the lattice parallel to the  $xz$ -plane located at  $y = \lfloor L/2 \rfloor$  ( $\lfloor \cdot \rfloor$  denotes the integer part). We check whether it contains a GS cluster which spans the plane in just a certain direction e.g.,  $z$ -direction. Therefore, we can obtain the probability  $P_s$  to have a spanning GS cluster at temperature  $T$ . We then measure the average mass of the largest spin-cluster,  $M$ . At each temperature, the averages are taken over  $10^2$  independent simulation runs and during each run another average is taken over  $10^5$  independent samples each of which is taken after  $L$  Monte Carlo steps [25]. This rather large number of averages is needed to obtain smooth curves close enough to the Curie point. The results are shown in Figs. 1 and 2 as a function of inverse temperature  $\beta$ .

As shown in Fig. 1, the curves  $P_s(\beta)$  computed for different cross sectional lattice sizes for sufficiently near sizes, cross at the same point very close to the Curie point, implying that the scaling dimension of the percolation probability is zero. This agrees with what is expected from scaling theory [4] which states that the  $P_s$  curves should have the form  $P_s(\beta) = P_s[(\beta/\beta_c - 1)L^{1/\nu}]$ . The exponent  $\nu$  characterizes the divergence of the correlation length  $\xi$  as the percolation threshold is approached,  $\xi \sim |\beta/\beta_c - 1|^{-\nu}$ . Note that here  $\xi$  is proportional to the spatial extent of the GS clusters in 2d slices of the 3d Ising model [26].

By utilizing the data collapse, it is possible to estimate the values of the exponent  $\nu$  and the crossing point of the curves  $\beta'_c$ . To measure the quality of the collapse of the curves we define a function  $S(\nu, \beta)$  as a function of the chosen values of  $\nu$  and  $\beta$  (the smaller  $S$  is indicative of a better quality of the collapse – see [19, 20] and appendix of [21]). We find its minimum  $S_{min} \sim 1.24$  for values  $\nu = 0.36(3)$  and  $\beta'_c = 1.0012(10)\beta_c$ , confirming the percolation threshold of the 2d GS clusters at the Curie

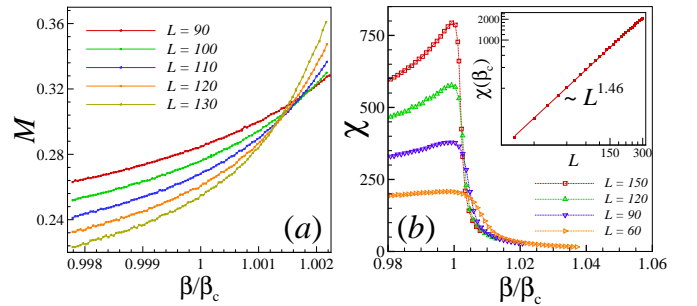


FIG. 2: (Color online) (a) The average mass of the largest GS cluster  $M$ , and (b) the mean cluster size  $\chi$  as a function of  $\beta$ . Inset: size dependence of  $\chi$  at  $\beta = \beta_c$ .

point. Applying these values for  $\nu$  and  $\beta'_c$ , rescaling of the data for different lattice sizes fall onto a universal curve (see upper inset of Fig. 1(a)). However crossing point of the curves is slightly different from  $\beta_c$ , but if one does not consider this discrepancy, the proper data collapse would not be achieved because, due to the relatively small value of  $\nu$ , the factor  $L^{1/\nu}$  would magnify this discrepancy along the  $x$ -axis and thus the curves do not collapse onto a single function. This effect will be more evident when one zooms in around zero on the  $x$ -axis. We find that the crossing point moves towards the Curie point for larger system sizes (Fig. 1(b)). Considering the  $P_s$  curve for  $L' = 40$  as a reference curve, we find that the crossing point of the other curves for different sizes with this reference curve i.e.,  $\beta'_c(L, L')$ , behaves like  $[(\beta'_c(L, 40)/\beta_c) - 1] \sim L^{-\omega}$ , with  $\omega = 1.02(5)$ , which is independent of  $L'$ . Therefore, to obtain a proper collapse even close enough to the crossing point, we need to measure  $\beta'_c$  with high precision which is possible for only two  $P_s$  curves. An example of such collapse is shown in the lower inset of Fig. 1(a), for system sizes  $L = 40$  and  $70$ . However, our estimation for the exponent  $\nu$  is not accurate and has to be reevaluated by considering the corrections-to-scaling effects.

In order to check that the coincidence between the percolation threshold  $\beta'_c$  of the 2d GS clusters and the Curie point  $\beta_c$  is not specific to the considered lattice geometry, i.e., SC structure, we repeated the Monte Carlo computations for a face-centered cubic (FCC) lattice. Note that both  $\beta'_c$  and  $\beta_c$  depend on lattice geometry. We find again their coincidence for the FCC lattice.

We have also computed the percolation strength  $M$ , as the order parameter in the percolation, and the mean cluster size  $\chi$  (Fig. 2). We find that, at the Curie point  $\chi$  scales as  $L^{\gamma'}$ , with  $\gamma' = 1.46(4)$ . These are indicative of a continuous transition of 2d GS clusters.

These scaling arguments suggest a fractal structure for 2d GS clusters, meaning that at  $\beta_c$  there exists a set of GS clusters and their surrounding loops at all scales.

In order to investigate manifestation of conformal invariance in the critical behavior of the GS clusters on the cross sections, we analyze statistical properties of the boundaries of these clusters and compare them with the SLE curves. We first measure the fractal dimension of the cluster boundaries and check the duality relation. The fractal dimension of SLE curves is given by  $d_f = 1 + \kappa/8$ , and the duality conjecture [8] states that the EP of SLE hulls for  $\kappa > 4$  looks locally as SLE curves but with a dual value  $\kappa' = 16/\kappa$ .

We undertook extensive Monte Carlo simulations with anisotropic geometry to obtain a reliable estimate of the fractal dimension at the Curie point  $\beta_c$  (the value of  $\beta_c$  has been determined to a high precision in Ref. [22]). We present the results of calculations for rather large system sizes of  $L_x \times L_y \times L_z$ , with  $L_y = L_z = L$ ,  $L_x = 4L$  and  $10 \leq L \leq 290$ . The periodic boundary condition was applied along all three directions. After equilibration, we collected a number of  $10^5$  ( $5 \times 10^4$ ) of independent spin

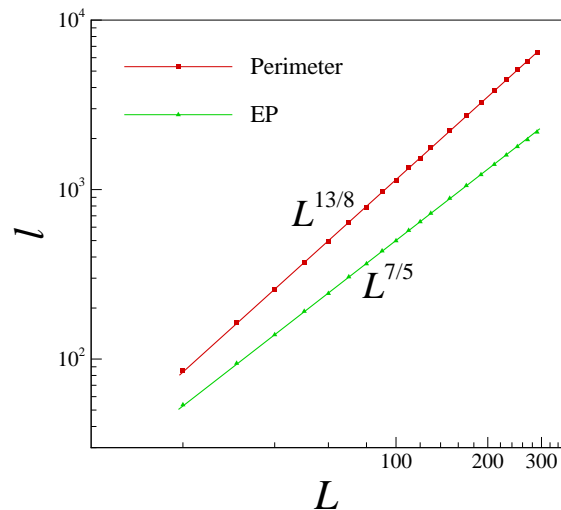


FIG. 3: (Color online) The average length of the perimeter (■) and EP (▲) of a spanning GS cluster versus the system size  $L$ , compared with ones for SLE<sub>5</sub> and SLE<sub>16/5</sub> curves (solid lines), respectively. The error bars are almost the same size as the symbols.

configurations on a planar cross section of the 3d sample located at  $y = \lfloor L/2 \rfloor$  for smallest (largest) system size. Each configuration was taken after the  $L_x$  Monte Carlo steps. We then identified all GS clusters on each cross section of a fixed size  $L$ , and marked all spanning clusters (if exist) along the  $z$ -direction. For each spanning cluster, a walker was applied to determine each of its perimeters which connect the lower boundary to the upper one along the  $z$ -direction. The walker was forced to start moving from a node on the dual lattice (which is also a square lattice) lied at the most left (right) site belonging to the spanning cluster on the lower boundary, by using the turn-right (left) *tie-breaking* rule [23] and thereby, for each size  $L$ , an ensemble of interfaces was obtained. It is shown in [23] that using these tie-breaking rules, one can obtain the interfaces on a square lattice without any ambiguity compatible with the conformal invariant properties of critical lattice models. According to each interface, the EP was also determined as the border of the corresponding interface after closing off all its boundary narrow passageways of lattice spacing  $a$ .

For fractal interfaces, their average length  $l$ , measured in units of lattice spacing  $a$  (which is set to unity here), scales as a function of the system size  $L$  as  $l \sim a(L/a)^{d_f}$  where  $d_f$  is the fractal dimension. Applying this relation for the ensemble of the perimeters and the EPs, we find their fractal dimensions equal to  $d_f = 1.621(10)$  and  $d'_f = 1.389(10)$ , respectively. These results give rise to  $\kappa = 4.96(8)$  and  $\kappa' = 3.11(8)$  for the perimeter and EP of a GS cluster, respectively, comparable with ones for SLE curves with diffusivity  $\kappa = 5$  and  $\kappa' = 16/5$ , which satisfy the duality relation (we find  $\kappa\kappa' = 15.42(65)$ , comparable

with the exact one  $\kappa\kappa' = 16$ ). To show this consistency, we have compared the results of our simulations with those predicted for SLE curves in Fig. 3. The exponent  $\delta' = 1.23(1)$  obtained in [13] for the hull of the GS clusters is also in a good agreement with our result  $\delta = 2/d_f = 2/(1 + \kappa/8) \sim 1.23077$  with  $\kappa = 5$ .

To verify further the consistency between the statistical behavior of the interfaces of GS clusters in a 2d cross section of the 3d Ising model and the SLE curves with  $\kappa = 5$  and  $\kappa' = 16/5$ , let us now examine their winding angle statistics which is predicted by the theory of SLE for critical interfaces [7]. We use the definition given in [24]. For each interface, an arbitrary winding angle is attributed to the first edge (which is taken to be zero here). The winding angle for the next edge is then defined as the sum of the winding angle of the present edge and the turning angle to the new edge measured in radians. It is shown that [24] the variance in the winding grows with the system size like

$$\langle \theta^2 \rangle = c + \frac{\kappa}{4} \ln L, \quad (1)$$

where  $c$  is a constant whose value is irrelevant. As shown in Fig. 4, the winding angle statistics of GS interfaces are in a good agreement with those of the corresponding SLE curves. We find that  $\kappa = 4.93(10)$  and  $\kappa' = 3.15(10)$ .

The point which has to be explained and discussed here is the seeming discrepancy between the exponents obtained from the direct percolation properties of the GS clusters and the ones obtained by analyzing the fractal properties of their hull and external perimeter. The latter study gives rise to a connection between statistical behavior of the boundaries of GS clusters in a 2d cross

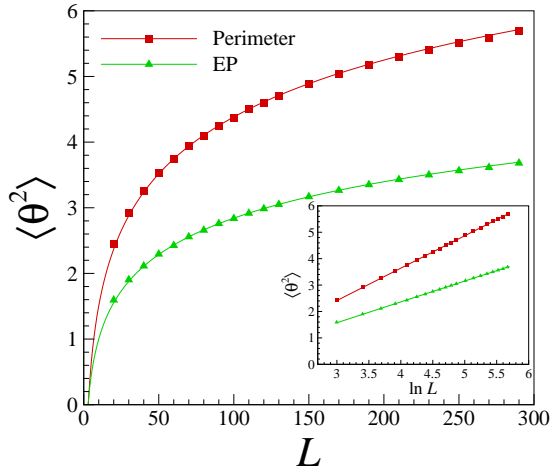


FIG. 4: (Color online) Variance of the winding angle for the perimeter (■) and EP (▲) of GS clusters on a 2d cross section of the 3d Ising model. The solid lines are set according to the Eq. (1) for comparison, with  $c \simeq -1.37$  and  $\kappa = 5$  for upper graph and with  $c \simeq -0.84$  and  $\kappa = 16/5$  for the lower graph. In the inset, the variance in semilogarithmic coordinates.

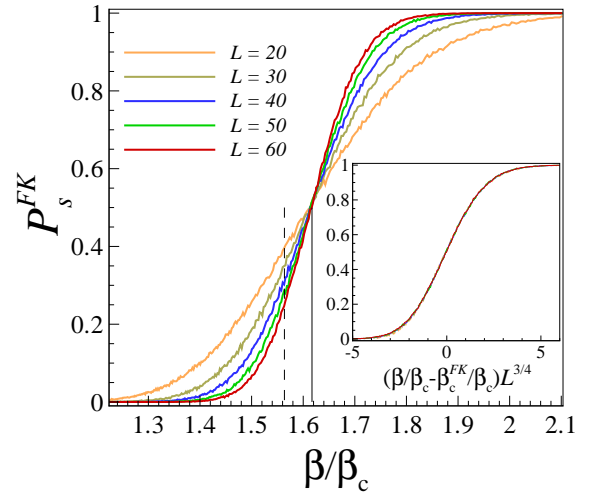


FIG. 5: (Color online) Percolation probability for FK clusters,  $P_s^{FK}$ , on a 2d cross section of 3d Ising model as a function of  $\beta$ , for different lattice size  $L$ . Inset: the data collapse with  $\nu = 4/3$  for 2d classical percolation, and  $\beta_c^{FK}/\beta_c = 1.617$ .

section of the 3d Ising model with those of FK clusters in a pure 2d tricritical Ising model, while the values of the geometrical exponents obtained in the first part of the paper are obviously not those predicted for tricritical Ising model at its thermal critical point. Although we do not have a full description of such discrepancy, its resolution seems to lie on natural difference between GS and FK clusters. Moreover, the notion of conformal invariance in the statistical behavior of the hull and external perimeter of GS clusters requires extraction of the statistics of the Loewner driving function and showing that it is a Brownian motion, which is very hard to do on small samples such as ours. These will be investigated in details in a future work.

So far, we have focused only on the statistical properties of GS clusters. We now present the results of the same study for the FK clusters built up on a 2d spin configuration by assigning a bond between each pair of nearest neighbor sites of the like spins with probability  $p = 1 - e^{-2\beta}$ . Our analysis indicates that the percolation transition of the FK clusters occurs at  $\beta_c^{FK}/\beta_c = 1.617(1)$  (shown by the vertical solid line in Fig. 5). This is obtained by computing the percolation probability shown in Fig. 5, with the same procedure as for GS clusters. We find that the critical behavior of these clusters is in the same universality class as the 2d critical percolation. As shown in the inset of Fig. 5, all curves fall well onto a universal curve with the same correlation exponent i.e.,  $\nu = 4/3$  as for classical bond percolation. The percolation threshold of 2d bond percolation on a square lattice is located at  $p = 1/2$  which is determined by the vertical dashed line in the Fig. 5, at  $\beta < \beta_c^{FK}$ , indicative of a nontrivial percolation transition at  $\beta_c^{FK}$ . The latter is expected due to the condensation of the



majority spins at low temperatures. The analysis of the statistical properties of the perimeter and EP of FK clusters will appear in the forthcoming paper.

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  - [26] The two point spin-spin correlation function in the original 3d Ising model is equal to the pair connectedness function of 3d FK clusters, i.e.,  $\langle s(x)s(y) \rangle = \langle \delta_{C_x, C_y} \rangle$ , which equals the probability that points  $x$  and  $y$  belong to the same FK cluster [18]. The corresponding correlation length of the 3d Ising model which is proportional to the spatial extent of the 3d FK clusters is characterized by the well-known exponent  $\nu \sim 0.63$ .